TWO STEP RUNGE-KUTTA-NYSTRÖM METHOD FOR SOLVING SECOND-ORDER ORDINARY DIFFERENTIAL EQUATIONS

By

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Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfillment of the Requirement for the Degree of Doctor of Philosophy

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DEDICATIONS

To

My beloved parents, Mr. Md Ariffin Md Nor and Madam Mahfuzah Abd Ghaffar,

my faithful husband, Major Mohd Safiee Idris Mat Ali (Amdias),

my loyal and beautiful princesses,

Ms. Syasya Syahmina Amdias,

Ms. 'Adlina Safiyy Amdias,

Ms. 'Aaliah Syakirah Amdias and

future Amdias's clan.

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfillment of the requirement for the Degree of Doctor of Philosophy

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Chairman: Professor Dato' Mohamed Bin Suleiman, PhD
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In this research, methods that will be able to solve the second order initial value problem (IVP) directly are developed. These methods are in the scheme of a multi-step method which is known as the two-step method. The two-step method has an advantage as it can estimate the solution with less function evaluations compared to the one-step method. The selection of step size is also important in obtaining more accurate and efficient results. Smaller step sizes will produce a more accurate result, but it lengthens the execution time.

Two-Step Runge-Kutta (TSRK) method were derived to solve first-order Ordinary Differential Equations (ODE). The order conditions of TSRK method were obtained by using Taylor series expansion. The explicit TSRK method was derived and its stability were investigated. It was then analyzed experimentally. The numerical results obtained were analyzed by making comparisons with the existing methods in terms of maximum global error, number of steps taken and function evaluations.

The explicit Two-Step Runge-Kutta-Nyström (TSRKN) method was derived with reference to the technique of deriving the TSRK method. The order conditions of TSRKN method were also obtained by using Taylor series expansion. The strategies in choosing the free parameters were also discussed. The stability of the methods derived were also investigated. The explicit TSRKN method was then analyzed experimentally and comparisons of the numerical results obtained were made with the existing methods in terms of maximum global error, number of steps taken and function evaluations.

Next, we discussed the derivation of an embedded pair of the TSRKN (ETSRKN) methods for solving second order ODE. Variable step size codes were developed and numerical results were compared with the existing methods in terms of maximum

global error, number of steps taken and function evaluations. The ETSRKN were then used to solve second-order Fuzzy Differential Equation (FDE). We observe that ETSRKN gives better accuracy at the end point of fuzzy interval compared to other existing methods.

In conclusion, the methods developed in this thesis are able to solve the system of second-order differential equation (DE) which consists of ODE and FDE directly.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk Ijazah Doktor Falsafah

KAEDAH RUNGE-KUTTA-NYSTRÖM DUA LANGKAH BAGI MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA PERINGKAT DUA

Oleh

LATIFAH BINTI MD ARIFFIN

Disember 2016

Pengerusi: Profesor Dato' Mohamed Bin Suleiman, PhD
Fakulti: Sains

Di dalam kajian ini, kaedah yang boleh menyelesaikan masalah nilai awal secara terus dibangunkan. Kaedah ini adalah di dalam skim multi-langkah di mana ia dikenali sebagai kaedah dua-langkah. Kaedah dua-langkah mempunyai kelebihan di mana ia boleh menganggar penyelesaian dengan kurang penilaian fungsi berbanding dengan kaedah satu-langkah. Pemilihan saiz langkah juga penting bagi memperolehi keputusan yang lebih jitu dan efisyen. Saiz langkah yang kecil akan menghasilkan keputusan yang lebih jitu, tetapi ia akan memanjangkan tempoh masa pelaksanaan.

Kaedah Runge-Kutta Dua Langkah (RKDL) diterbitkan bagi menyelesaikan Persamaan Pembezaan Biasa (PPB) peringkat satu. Syarat peringkat bagi kaedah RKDL tak tersirat diperolehi dengan menggunakan kembangan siri Taylor. Kaedah RKDL tak tersirat diterbitkan dan kestabilannya dikaji. Ia kemudiannya dianalisa secara eksperimen. Keputusan berangka yang diperolehi dianalisa dengan membuat perbandingan bersama kaedah-kaedah sedia ada berdasarkan kepada ralat global maksimum, bilangan langkah dan penilaian fungsi.

Kaedah Runge-Kutta-Nyström Dua Langkah (RKNDL) tak tersirat diterbitkan mengikut teknik seperti penerbitan kaedah RKDL. Syarat peringkat bagi kaedah RKNDL juga diperolehi dengan menggunakan kembangan siri Taylor. Strategi pemilihan parameter bebas juga dibincangkan. Kestabilan kaedah-kaedah ini juga dikaji. Kaedah RKNDL tak tersirat ini kemudiannya dianalisa secara eksperimen dan perbandingan dilakukan bersama kaedah-kaedah sedia ada berdasarkan kepada ralat global maksimum, bilangan langkah dan penilaian fungsi.

Seterusnya kami membincangkan penerbitan kaedah Benaman RKNDL (BRKNDL) bagi menyelesaikan PPB peringkat dua. Kod langkah berubah dibangunkan dan keputusan berangka dibandingkan dengan kaedah-kaedah sedia ada berdasarkan kepada ralat global maksimum, bilangan langkah dan penilaian fungsi. Kaedah BRKNDL ini

kemudiannya digunakan untuk menyelesaikan Persamaan Pembezaan Kabur (PPK). Kami mendapati bahawa kaedah BRKNDL memberi kejituan yang lebih baik pada titik hujung selang kabur berbanding dengan kaedah-kaedah sedia ada.

Kesimpulannya, kaedah-kaedah yang diterbitkan di dalam tesis ini dapat menyelesaikan sistem persamaan pembezaan (PP) yang merangkumi PPB dan PPK peringkat dua secara terus.

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LIST OF ABBREVIATIONS

BVP	Boundary Value Problem
DE	Differential Equation
ERK3(2)D	A second-order three-stage explicit RK method embedded into third-order three-stage RK method derived by Dormand (1996).
ERK4(3)B	A third-order four-stage explicit RK method embedded into fourth-order four-stage RK method derived by Butcher (1987).
ERK4(3)F	A third-order four-stage explicit RK method embedded into fourth-order four-stage RK method derived by Fehlberg (1970).
ETSRKN	Embedded Two-Step Runge-Kutta-Nyström
ETSRKN3(2)	The two-stage second-order embedded in two-stage third-order TSRKN method
ETSRKN4(3)	The three-stage third-order embedded in three-stage fourth-order TSRKN method
FCN	Number of Function Evaluations
FDE	Fuzzy Differential Equation
FETSRKN	Fuzzy Embedded Two-Step Runge-Kutta-Nyström
FIVP	Fuzzy Initial Value Problem
H-derivative	Hukuhara-Differentiability
HPC	High Performance Computing Machine
IVP	Initial Value Problem
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
PLTE	Principal Local Truncation Error
RK	Runge-Kutta
RK3(3)B	The three-stage third-order explicit RK method derived by Butcher (1987)
RK3(3)D	The three-stage third-order explicit RK method derived by Dormand (1996)

RK4(3)B	The four-stage third-order embedded in four-stage fourth-order RK method derived by Butcher (1987)
RK4(3)F	The four-stage third-order embedded in four-stage fourth-order RK method derived by Fehlberg (1970)
RKN	Runge-Kutta-Nyström method
RKN3(3,12,3)	A three-stage third-order RKN method with dispersive order twelve and dissipative order three derived by van der Houwen and Sommeijer (1987).
RKN4(4,10,5)	A four-stage fourth-order RKN method with dispersive order ten and dissipative order five derived by van der Houwen and Sommeijer (1987)
TSRK	Two-Step Runge-Kutta method
TSRK2(3)	The two-stage third-order explicit TSRK method
TSRKN	Two-Step Runge-Kutta-Nyström method
TSRKN2(3)	The two-stage third-order explicit TSRKN method
TSRKN3(4)	The three-stage fourth-order explicit TSRKN method
$C_2(p)$	Simplifying conditions for m −stage TSRKN method
$B_2(p)$	Simplifying conditions for m −stage TSRKN method
$B'_2(p)$	Simplifying conditions for m −stage TSRKN method

CHAPTER 1

INTRODUCTION

1.1 Introduction

Many problems in engineering and science can be formulated in terms of differential equations. These problems arise in mechanical and electrical systems, celestial and orbital mechanics, molecular dynamics, seismology and many other engineering problems. A differential equation is defined as an equation that involves a relation between an unknown function with one or more of its derivatives. Basically, a differential equation involving only ordinary derivatives with respect to single independent variable is called Ordinary Differential Equation (ODE). Meanwhile, a differential equation involving partial derivatives with respect to more than one independent variable is called Partial Differential Equation (PDE). Furthermore, ODE may be classified as either initial-value problem (IVP) or boundary-value problem (BVP).

The most discussed IVP are in class of the first and second order. These problems can be solved analytically when they are linear. However, very few nonlinear problems can be solved analytically. Thus, one must rely on numerical scheme to solve these problems. Methods for solving IVP numerically are classified into two schemes, which are the one-step method and the multi-step method. Many numerical one-step methods have been developed such as Euler method, Runge-Kutta (RK) method and Taylor series method where these methods are used to solve the first order IVP directly. These methods are also being used to solve the second order IVP indirectly by reducing it to the first order equations system. Even though this approach is easy to implement but it will enlarge the equation system and will increase the cost for the process.

1.2 Objectives of the Thesis

The main objective of this thesis is to develop a two-step Runge-Kutta-Nyström (TSRKN) method with a constant step-size and a variable step-size for solving special second-order IVP directly. The objectives can be accomplished by:

1. Develop the order conditions for two-step Runge-Kutta (TSRK) by using Taylor series expansion, derive the TSRK method and implement the method to solve first order IVP using constant step-size code;
2. Develop the order conditions for TSRKN by using Taylor series expansion, derive the TSRKN method and implement the method to solve special second order IVP using constant step-size code;
3. Investigate the stability and convergence of the derived TSRK and TSRKN methods;

4. Derive the embedded two-step Runge-Kutta-Nyström (ETSRKN) method and implement the method to solve special second order IVP using variable step-size code;
5. Solve second order fuzzy differential equations (FDE) by using ETSRKN method that had been derived previously to show the ability of the method to solve other type of DEs.

1.3 Outline of the Thesis

In Chapter 1, a brief introduction on differential equations and the application of numerical methods for solving different types of differential equations are given.

In Chapter 2, a brief introduction to IVP and Taylor series expansion were given. Then earlier researches related to TSRK and TSRKN methods for solving first order ODE and, second order ODE and FDE were provided. The stability properties for these methods were also presented. Some basic definitions and theorems related to the subject were also given. FDE and FIVP were discussed at the end of this chapter.

In Chapter 3, we start with the development of the order conditions from order one up to order four for TSRK method by using Taylor series expansion. Based on the order conditions obtained, we derived the two-stage third-order TSRK explicit method. The strategies of choosing the free parameters of the method for developing a more accurate computed solution are also discussed. The convergence of the method is proven and the stability regions of the method are presented. To illustrate the efficiency of the method, a number of tested problem are validated and the numerical results are compared with existing RK method of the same order derived by Dormand (1996) and Butcher (1987). Stability interval for all methods will also be presented.

Chapter 4 will discuss the development of order conditions from order one up to order four for TSRKN method by using Taylor series expansion. A two-stage third-order and three-stage fourth-order explicit TSRKN method were derived using the same strategy as found in Chapter 3. Several problems are solved and their numerical results are compared with the existing RK method of the same order. For existing RK method of order three, comparisons are made with methods derived by Butcher (1987) and van der Houwen and Sommeijer (1987). Likewise, comparisons are made with RK method of order four derived by Lambert (1991) and RKN method of order four derived by van der Houwen and Sommeijer (1987). Stability interval for all methods will also be presented.

For variable step-size, the development of an embedded pair for explicit TSRKN (ETSRKN) methods based on formulas derived in Chapter 4 are discussed in Chapter 5. The choices of free parameters in obtaining the optimized pair are also discussed. Special second-order IVP are solved including oscillating problems. Numerical results and their performances are presented. For the new ETSRKN 3(2) pair, comparisons are made with an existing embedded RK 3(2) pair derived by Dormand (1996).

Meanwhile, for the new ETSRKN 4(3) pair, comparisons are made with an existing embedded RK 4(3) pair derived by Butcher (1987) and Fehlberg (1970). The ETSRKN 4(3) pair method then is adapted for solving second-order fuzzy differential equations. Two fuzzy problems are solved and their numerical results are compared with the existing embedded RK method.

Finally, the summary of the whole thesis, conclusions and future research are given in Chapter 6.

1.4 Motivation and Contribution of the Thesis

Many differential equations which appear in practice are systems of second order IVP. This system can be reduced into first order differential equations of doubled dimension. In this study we are focusing on solving the second order IVP directly. Our proposed method able to solve the second order problems directly that is TSRKN method. We focus only on the explicit type of method. In addition to the implementation of the method, accuracy and stability are two other factors used for judging the efficacy of the methods.

1.5 Scope of the Thesis

This study concentrate on the development of new coefficient and efficient codes that are based on explicit TSRKN methods for numerical solution of IVP. These methods will then be used for solving system of second order ODEs directly for both constant and variable step size mode. The properties of this method will be analyzed in terms of order, consistence and convergence. Our main motivation is to reduce the number of steps taken in solving second order IVP directly by using this method as well as to reduce the number of function evaluations where it will ensure cost efficiency.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

In this chapter, we begin with a brief introduction to IVP for second-order ODE in section 2.2. Next, Taylor series expansion were defined in section 2.3. The literature review for the TSRK method for solving first-order IVP is presented in section 2.4. Meanwhile, the literature review for the TSRKN methods for solving special second-order IVP of ODE is presented in section 2.5. Section 2.6 defined the stability properties of both method. The TSRKN method were then proposed to solve the fuzzy differential equations with some modification in section 2.7 to solve Fuzzy Initial Value Problem (FIVP) in section 2.8.

2.2 Initial Value Problem

The initial value problem for a system of s special second order ODE is defined as

$$y'' = f\big(x, y(x)\big), \quad y(x_0) = y_0, \quad y'(x_0) = y_0 \tag{2.1}$$

where $y(x) = [y_1(x), y_2(x), \dots, y_s(x)]^T, \quad y'(x) = \big[y'_1(x), y'_2(x), \dots, y'_s(x)\big]^T$

$$f(x,y) = [f_1(x,y), f_2(x,y), \dots, f_s(x,y)]^T, \quad x \in [a,b],$$

$y_0 = [y_{01}, y_{02}, \dots, y_{0s}]^T$ and $y'_0 = \big[y'_{01}, y'_{02}, \dots, y'_{0s}\big]^T$ are the vectors of initial conditions.

Theorem 2.1 *(Existence and Uniqueness)*
Let $f(x,y)$ be defined and continuous for all points (x,y) in the region D defined by $a \leq x \leq b, -\infty < y < \infty$, a and b finite, and let there exist a constant L such that, for every x, y, y^* such that (x,y) and (x,y^*) are both in region D, where

$$|f(x,y) - f(x,y^*)| \leq L|y - y^*|. \tag{2.2}$$

Then, if y_0 is any given number, there exist a unique solution $y(x)$ of the initial value problem (2.1), where $y(x)$ is continuous and differentiable for all (x,y) in D.

The requirement (2.2) is known as Lipschitz condition, and the constant L is known as a Lipschitz constant. For the proof of Theorem 2.1, see Henrici (1962). In this work, we shall assume the conditions of the theorem are satisfied, hence establishing the existence of a unique solution of (2.1).

2.3 Taylor Series Expansion

Given that the function $y(x)$ is sufficiently differentiable, $y(x+2h)$ can be expended in a Taylor's series form

$$y(x+2h) = y(x) + 2hy'(x) + \frac{(2h)^2}{2!}y"(x) + \cdots + \frac{(2h)^p}{p!}y^p(x) + \cdots \tag{2.3}$$

where $y^p(x) = \frac{d^p y}{dx^p}$ with $p = 1,2, \ldots$. Similarly, we write the Taylor's series expansion of $y(x_n + 2h)$ as follows

$$y(x_n+2h) = y(x_n) + 2hy'(x_n) + \frac{(2h)^2}{2!}y"(x_n) + \cdots + \frac{(2h)^p}{p!}y^p(x_n) + \cdots \tag{2.4}$$

The series on the right-hand side of (2.4) has an infinite number of terms in order to preserve the equality, and is not a practical formula for evaluating $y(x_{n+2})$. In practice, all terms up to and including that involving h^p are included, that is

$$\begin{aligned} y(x_{n+2}) &= y(x_n + 2h) \\ &= y(x_n) + 2hy'^{(x_n)} + \frac{(2h)^2}{2!}y''(x_n) + \cdots + \frac{(2h)^p}{p!}y^{(p)}(x_n) + 2h^{p+1}R_{p+1}(\xi_n) \end{aligned} \tag{2.5}$$

where $R_{p+1}(\xi_n)$ is the remaining term with $x_n \le \xi_n \le x_n + 2h$, approximated by the following truncated series

$$\begin{aligned} y(x_{n+2}) &= y(x_n + 2h) \\ &= y(x_n) + 2hy'(x_n) + \frac{(2h)^2}{2!}y"(x_n) + \cdots + \frac{(2h)^p}{p!}y^{(p)}(x_n) + O(h^{p+1}). \end{aligned} \tag{2.6}$$

Equation (2.6) is the Taylor series method of order p, y_n is taken to be the estimate of the exact value $y(x_n)$. From (2.6), generally an explicit two-step method can be written as

$$y_{n+2} = y_{n+1} + 2h\emptyset\big(x_{n,}y(x_n), h\big) \tag{2.7}$$

where $\emptyset(x, y, h)$ is a function of arguments x, y, h and in addition, it depends on the right-hand side of (2.1). The function $\emptyset(x, y, h)$ is called the increment function. The true value $y(x_n)$ will satisfy

$$y(x_{n+2}) = y(x_{n+1}) + 2h\emptyset\big(x_{n,}y(x_n), h\big) + T_n \tag{2.8}$$

where T_n is the truncation error.

Definition 2.1 *The method (2.7) is said to have order p if p is the largest integer that*

$$y(x + 2h) - y(x + h) - 2h\emptyset(x, y(x), h) = O(h^{p+1}) \tag{2.9}$$

where $y(x_n)$ is the analytical solution.

2.4 Two-Step Runge-Kutta (TSRK) Method

Consider the initial value problem for a system of ordinary differential equation (ODE)

$$y'(x) = f\big(x, y(x)\big), \quad x \in [a, b], \quad y(x_0) = y_0, \tag{2.10}$$

where the function $f: \mathbb{R}^q \to \mathbb{R}^q$ is assumed to be sufficiently smooth. These methods form a subclass of general linear methods considered by Butcher (1987) and are defined by

$$\begin{aligned} y_{i+2} &= (1-\theta)y_{i+1} + \theta y_i \\ &\quad + h\sum_{j=1}^{m} v_j f\big(x_i + c_j h, Y_i^j\big) + w_j f\big(x_{i+1} + c_j h, Y_{i+1}^j\big), \\ Y_i^j &= y_i + h\sum_{s=1}^{m} a_{js} f(x_i + c_s h, Y_i^s), \quad j = 1, \dots, m, \\ Y_{i+1}^j &= y_{i+1} + h\sum_{s=1}^{m} a_{js} f(x_{i+1} + c_s h, Y_{i+1}^s), \quad j = 1, \dots, m, \end{aligned} \tag{2.11}$$

$i = 1,2, \dots, n-1$, $h = \frac{b-a}{n}$, where the starting values y_0 and y_1 are assumed to be given (Jackiewicz and Renaut, 1995).

It is convenient to represent (2.11) using the following Butcher table of coefficients:

Table 2.1: Butcher table for an explicit TSRK formula

$$
\begin{array}{c|ccccc}
c_2 & a_{21} & & & & \\
c_3 & a_{31} & a_{32} & & & \\
\vdots & \vdots & \vdots & \ddots & & \\
c_m & a_{m1} & a_{m2} & \cdots & a_{m\,m-1} & \\
\hline
\multirow{2}{*}{θ} & v_1 & v_2 & \cdots & v_{m-1} & v_m \\
 & w_1 & w_2 & \cdots & w_{m-1} & w_m
\end{array}
$$

where

$$c_i = \sum_{j=1}^{i-1} a_{ij}\,, i = 1,2, \dots, m, \tag{2.12}$$

and

$$\sum_{j=1}^{m} \left(v_j + w_j\right) = 1 + \theta. \tag{2.13}$$

The TSRK methods were first introduced by Byrne and Lambert in 1966. These two step methods are different from the classical RK methods where the evaluations of f in equation (2.10) made at the previous point were used along with those made at the current point in order to obtain the solution at the next point. They present a method having local accuracy $O(h^m)$ but requiring only $m-1$ derivative evaluations. They observed that these methods are consistent with the IVP and shown to be convergent to the exact solution of the IVP.

Jackiewicz et al. (1991) studied the implicit TSRK and derived the order conditions. Semi implicit TSRK was also constructed but no numerical results were presented for both types of method. In 1995, Jackiewicz et al. then analyzed the explicit formula for TSRK. They discovered that for order $p \leq 5$, the minimal number of stages for explicit TSRK method of order p is equal to the minimal number of stages for explicit RK method of order $p-1$. For example, explicit TSRK method of order three only needs two stages compared to explicit RK method of order three which requires three stages. Meanwhile, Jackiewicz and Tracogna (1995) developed the general order conditions for a general class of TSRK. They derived the order conditions for TSRK by using

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